# **Copernicus FICE 2025**

**Training on** 

In situ Ocean Colour Above-Water Radiometry towards Satellite Validation

## ThoMaS match-up toolkit

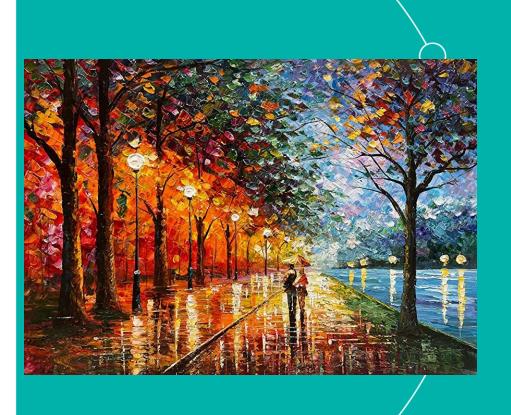
Juan Gossn EUMETSAT











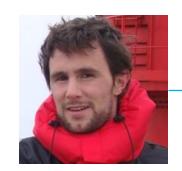
- What's ThoMaS? Scope
- Some background
- Usage
- Pre-requisites
- Getting the code
- Setting the environment
- Required inputs
- Run the code: examples

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ThoMaS is a toolkit developed to create **matchups** of biogeophysical **insitu data** with **satellite ocean colour products** from **Sentinel-3 OLCI (S3/OLCI)**.

in SeaBASS format

Standard products from NASA's OBPG also supported Others easily configurable, if netCDF or series of netCDFs



EUMETSAT colleague and friend Thomas Flament gave the name to the code after a joke

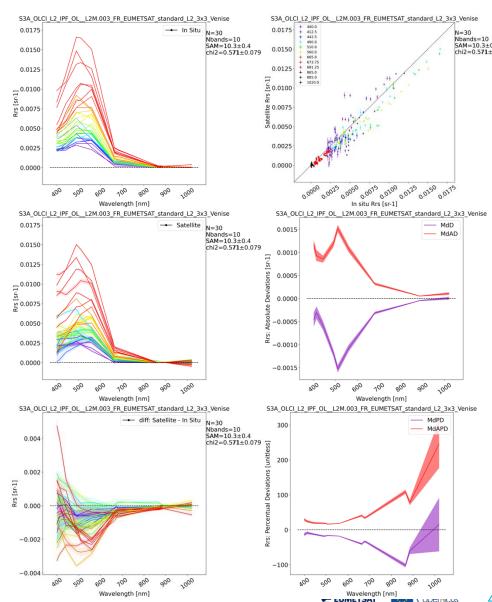
### What's ThoMaS? Scope

#### After running **ThoMaS**, you will get:

- → Insitu data "transformed" to match satellite (spectral convolution, bandshifting, spectral reconstruction, BRDF...).
- → Satellite data (L1B TOA radiance or L2 BOA water reflectance) from **EUMETSAT Data Store** and **NASA OBPG** (reprocessed/operational) matching spatially/temporally your insitu.
- > Extractions of satellite data centred at lat/lon of insitu of user-defined size (3x3, 5x5..).
- → Statistics of extractions following EUMETSAT's or any user-defined matchup protocol.
- → Merging of simultaneous (spatially-temporally) insitu-satellite pairs, temporal interpolation, and statistics of matchups.

#### $\rightarrow$ Outputs:

- → **NetCDF 4** files: SatData, minifiles, Extraction Data Base files, In situ Data Base file, Matchup Data Base files.
- → CSV: summarizing satellite extraction statistics and matchup statistics.
- → **PNG**: Standardised output plots.





#### Contributions and testers

- Essentially Juan is developing the code, but:
- Ilaria Cazzaniga (JRC) and Malcolm Taberner (EUMETSAT) developed the first match-up database workflow at EUMETSAT. Took many ideas and the main concept from this.
- Ewa Kwiatkowska and David Dessailly continuously support the development and the concept.
- Hayley Evers-King and Ben Loveday (EUMETSAT) contribute a lot to the code consolidation, user support, training, jupter notebooks, and testing
- Eleni Kalogeraki (ECMWF) developed the first version of the GUI as part of a 6-month internship at FUMFTSAT.
- Anna E. Wyndle di Paola, James G. Allen and Dirk Aurin (NASA) contributed to incorporate PACE.
- Frederic Melin (JRC) ran a preliminary verification with his own independent matchup workflow with identical results.
- Testers:
  - Pietro Sciuto (JRC)
  - The FICE 2024 and 2025 trainees ©

#### •

#### Motivation for having ThoMaS

- 1. Well documented, suited also for a first approach to the matchup exercise for those who are new to the matchup exercise.
- 2. It's publicly available, free and open to scrutiny: it serves for the purpose of converging to a standard matchup practice.
- 3. It supports the most commonly used matchup protocols in the OC community.
  - → e.g. of existing ones: EUMETSAT's, Bailey & Werdell 2006, Zibordi 2009, Copernicus SVC\_VIS
  - → Versatile: new matchup protocols can be easily added via configuration files.
  - → It contains an easy syntax to create new quality flags based on simple relations between products.
- 4. It deals (under some assumptions) with propagation of uncertainties to the performance metrics (using a Monte-Carlo approach).
- 5. Already supports some of the most commonly used OC satellite missions
  - → Currently supports Sentinel-3 (standard) L1B, L2, MODIS L2 (standard), VIIRS L2 (standard), SeaHawk L2 (standard) and PACE L2 (standard)
  - → Versatile: new types of satellite products can be easily added via configuration files (depending on mission, processor and processing baseline).



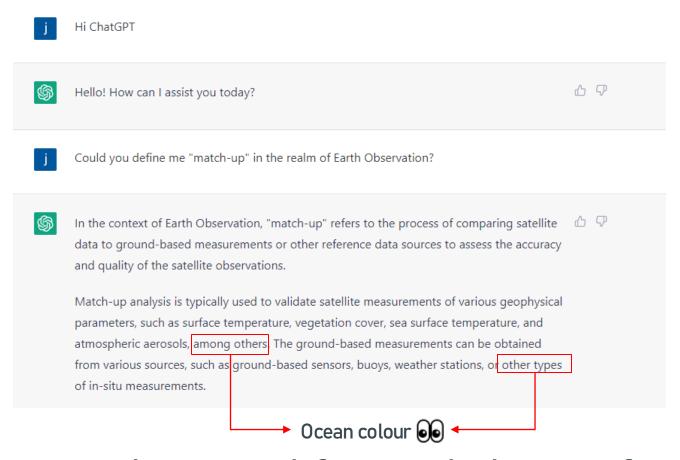
# ThoMaS is still not fully validated and is still under development ...

- 1. If you use it to run your match-up exercise, you are responsible to verify the results! Reporting back and working with us on improvements and troubleshooting is appreciated.
- 2. The policy of garbage-in garbage-out applies to ThoMaS: you must know well your insitu data, the satellite product, and make sure that you are comparing "apples" to "apples". Also, that your satellite pixels are sufficiently away from land, and rationally choose your extraction size, time difference tolerance, among many others.
- 3. ThoMaS does not deal with uncertainties coming from spatial and temporal collocation of insitu and satellite data beyond very standard QC (e.g. a maximum time tolerance window, a choice of window size, and a simple temporal interpolation). In other words, the problem of spatial and temporal autocorrelation of the Rrs signal (and any other OC product) is not yet dealt within ThoMaS.
- 4. ThoMaS cannot still compute match-up statistics of a given insitu-satellite set with varying satellite extraction sizes.
- 5. The uncertainty of the satellite component is only based on the inter-pixel variability (pixel-by-pixel uncertainties in the satellite component are still ignored in ThoMaS).
- 6. The uncertainties of the BRDF step are not propagated.
- 7. ThoMaS won't do an A/C of your satellite data!
- 8. Many other disclaimers (working on many of these ②), but I hope it still proves useful!



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• What is a match-up according to **ChatGPT** [2023]?



I You MADE THIS?

Chat GPT



Of course we have much more to define... and take care of...

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#### • What is a match-up according to **ChatGPT** [2025]?

Hi there! © How can I help you today?

Can you define a "match-up" in the realm of Earth

#### Certainly!

In the realm of Earth Observation (EO), a "match-up" refers to a coincidence or alignment I more datasets—typically from different sensors, platforms, or measurement techniques—the same target (usually a specific location on Earth) at nearly the same time and under comp conditions.

#### More formally:

A match-up is a spatiotemporal pairing between measurements (e.g., satellite, airborne, i data) that allows for direct comparison, validation, calibration, or data fusion.

#### Key Components of a Match-up:

#### Spatial Collocation

The observations must refer to the same geographic area, often defined within a specific radius or pixel size.

#### 2. Temporal Collocation

The observations must occur within a defined time window (e.g., within  $\pm 1$  hour) to ensure the measured environmental conditions are consistent.

#### Measurement Comparability

The observed quantities should be comparable (e.g., Sea Surface Temperature, Aerosol Optical Depth), with harmonized units and possibly corrected for known biases or differences in measurement geometry.

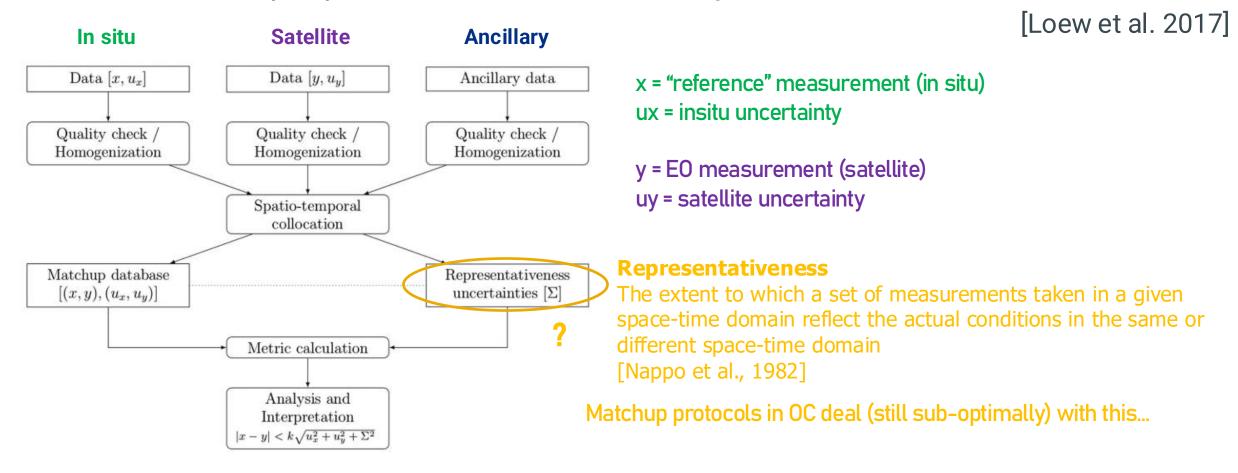
#### **Common Use Cases:**

- Satellite vs. In-situ Validation

  Comparing satellite data (e.g., ocean color) with ground-truth data from buoys or ships.
- Sensor Intercomparison
   Matching data from two different satellites to ensure consistency (e.g., MODIS vs. VIIRS).
- Data Assimilation and Fusion
   Combining different observations (e.g., satellite vodel outputs) to improve spatial/temporal coverage and accuracy.

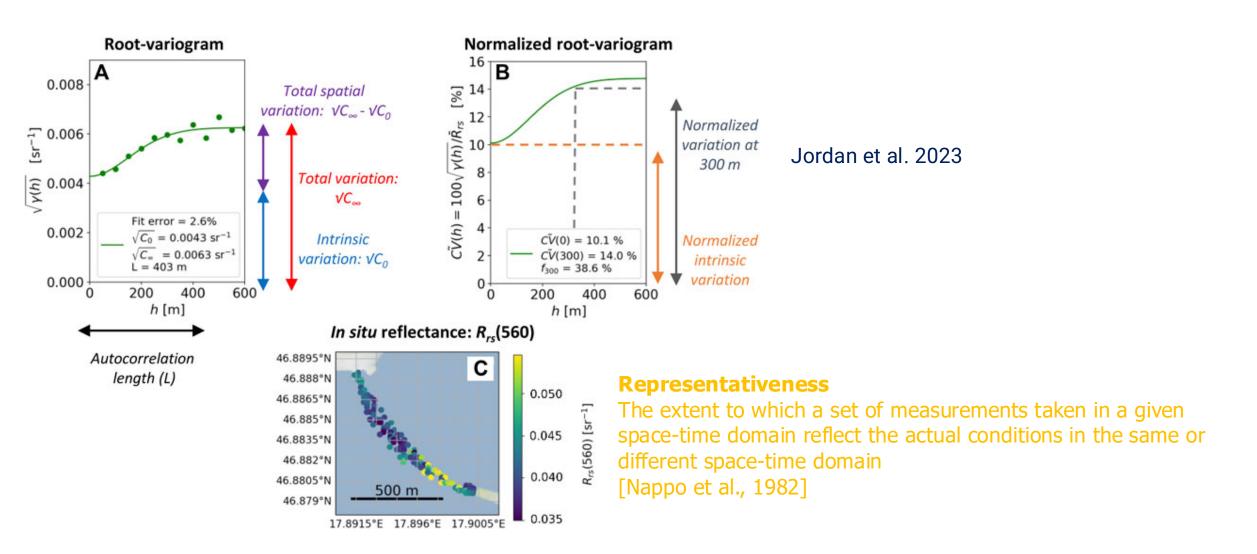


- The EO data are in practice rarely fully traceable, for instance, because fundamental
  calibrations done in the laboratory prelaunch cannot be repeated in space.
- Consequently the comparison against reference measurements in a validation exercise is
  often the only way to link the EO data back to an agreed standard.





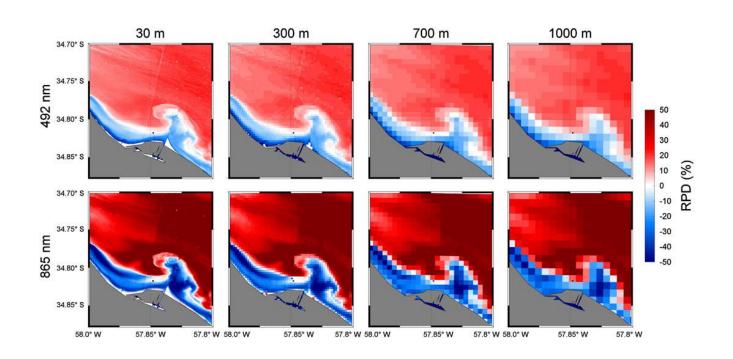
# Some background: match-ups, a note on spatial/temporal homogeneity



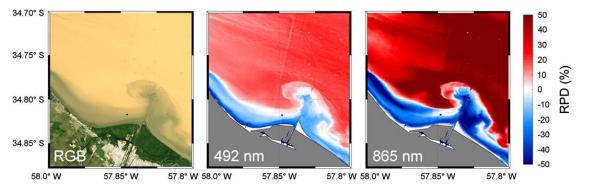


# Some background: match-ups, a note on spatial/temporal homogeneity

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Dogliotti et al. 2024



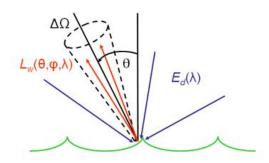
#### Representativeness

The extent to which a set of measurements taken in a given space-time domain reflect the actual conditions in the same or different space-time domain [Nappo et al., 1982]

**Definition of Rrs** 

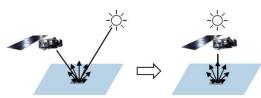
 $R_{ ext{ iny IS}}( heta,\phi,\lambda) \equiv rac{L_w\left( ext{in air}, heta,\phi,\lambda
ight)}{E_d\left( ext{in air},\lambda
ight)}$  $({\rm sr}^{-1})$  .

3A OLCI L2 IPF-Coll4 OL L2M.004 FR EUMETSAT standard L2 3x3 Optically Complex



00 Web Book, Mobley, Boss & Roesler

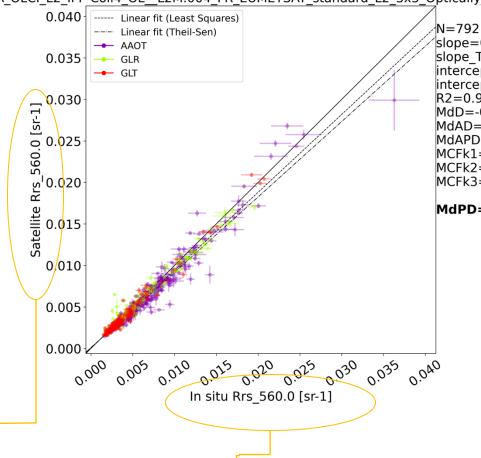
**BRDF** correction:



D'Alimonte et al. Morel et al. 2002 supported in ThoMaS

Are we comparing with ??

- → What is the <u>definition</u> of <u>Rrs?</u>
- → Are these two compatible "spectrally"? → convolution/band-shifting
- → Are these two compatible "directionally"? → BRDF correction



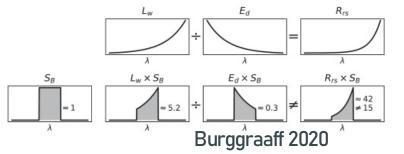
 $slope=0.938\pm0.015$ slope TS=0.9074±0.0053 intercept=0.00006±0.00008 intercept TS=0.00011±0.00005 R2=0.9738±0.0034 MdD=-0.00025±0.00002  $MdAD=0.00041\pm0.00001$ MdAPD=9.20±0.29 MCFk1=0.**Band-shifting (to pair multispectral to multispectral)** MCFk2=0.85MCFk3=0.97  $\mathbf{MdPD=-5.51\pm0.3} \ R_{RS}^{e} \left(\lambda_{i} \rightarrow \lambda_{t}\right) = R_{RS}^{f} \left(\lambda_{t}\right) \frac{R_{RS} \left(\lambda_{i}\right)}{R_{RS}^{f} \left(\lambda_{i}\right)}$ 

Melin & Sclep 2015 supported in ThoMaS

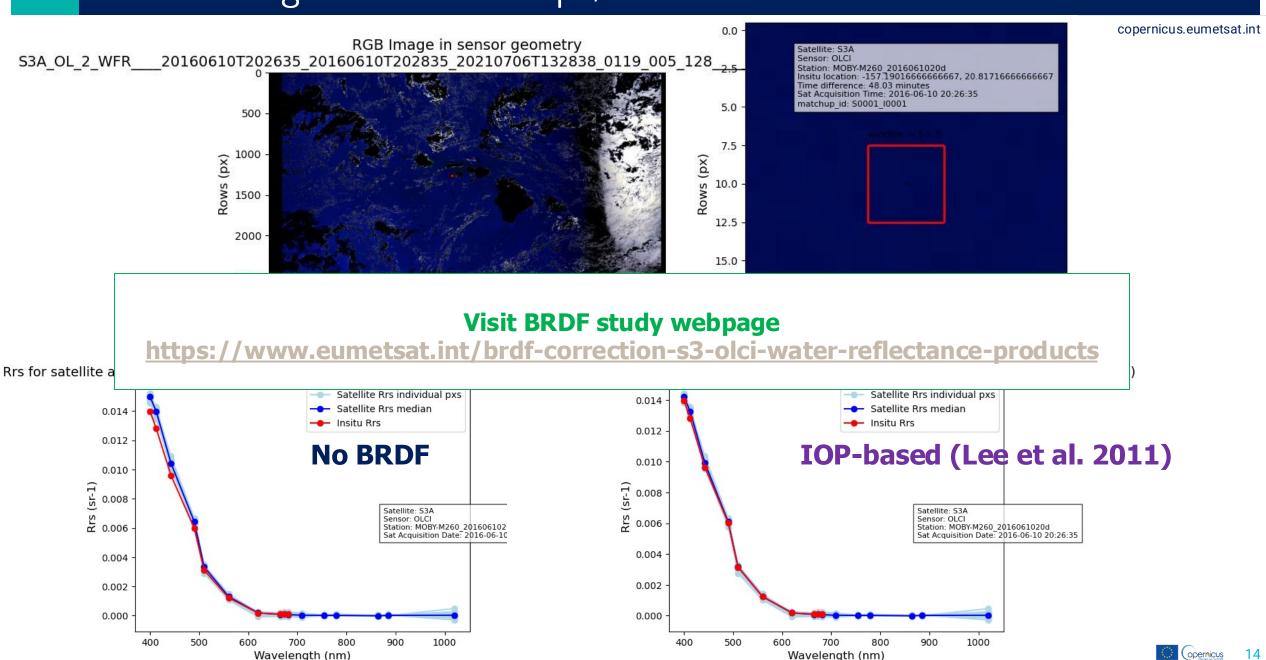
PACE: Spectral reconstruction

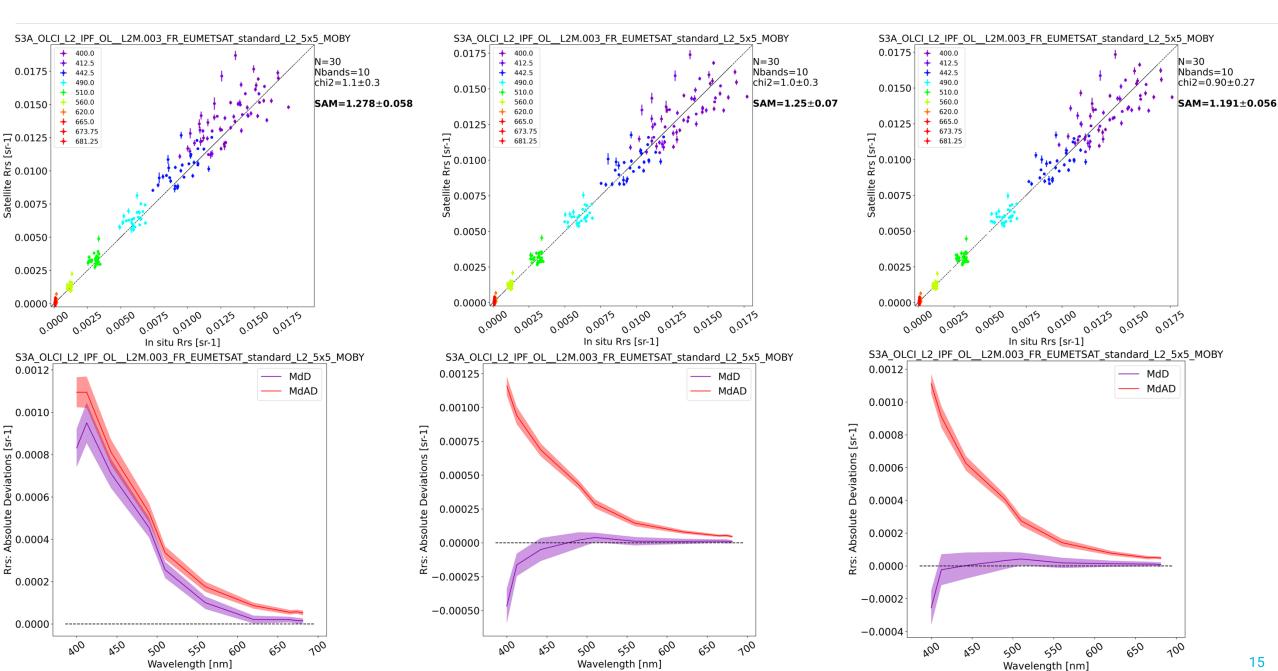
Talone, Zibordi, Pitarch 2024, recently added

#### Spectral convolution



#### Some background: match-ups, a note on BRDF correction





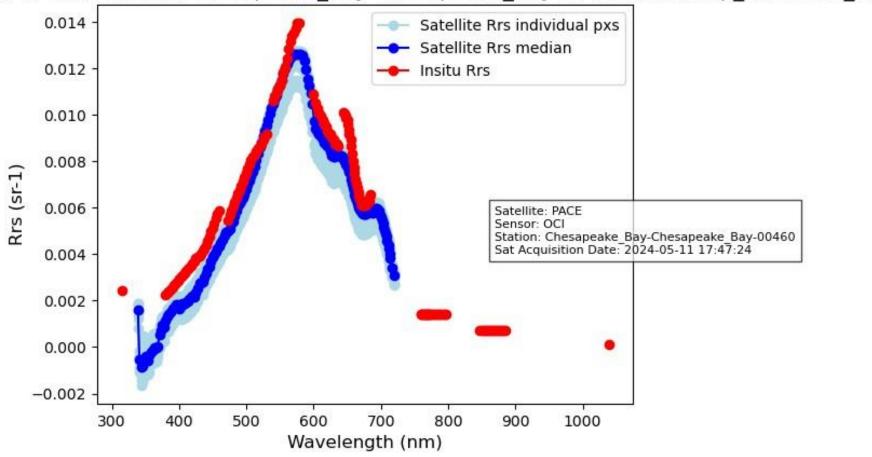


## Some background: match-ups (spectrally matching insitu to satellite)

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Melin & Sclep 2015 band-shifting method not applicable for hyper 2 hyper spectral matching

Rrs for satellite and in-situ (Station: Chesapeake Bay-Chesapeake Bay-00460, matchup id: S0022 10461)





# Some background: match-ups (spectrally matching insitu to satellite)

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Tried Talone, Zibordi and Pitarch 2024 method

#### This method:

- Finds the best 3 matches from a set of exhaustive hyperspectral Hydrolight simulations, using a selected set of multispectral bands.
- Establishes a blending approach in a way that the resulting reconstructed spectrum coincides exactly with the insitu original spectrum at the original multispectral bands and takes the spectral dependence of these best 3 matches in the intermediate "query" bands.

Validated with a concurrent hyperspectral in situ instrument, showing relative differences typically < 5 % between modelled and measured values.

IEEE GEOSCIENCE AND REMOTE SENSING LETTERS, VOL. 21, 2024

6002105

# On the Application of AERONET-OC Multispectral Data to Assess Satellite-Derived Hyperspectral $R_{rs}$

Marco Talone<sup>®</sup>, Senior Member, IEEE, Giuseppe Zibordi<sup>®</sup>, and Jaime Pitarch<sup>®</sup>

Abstract—The potential for applying in situ multispectral  $R_{rs}$ data from the Ocean Color component of the Aerosol Robotic Network (AERONET-OC) to validate satellite-derived ocean color hyperspectral  $R_{rs}$  products was investigated in the 400–700 nm interval. The analysis was performed using a comprehensive dataset of simulated hyperspectral  $R_{rs}$  in combination with an algorithm designed to reconstruct hyperspectral  $R_{rs}$  from multispectral ones. Results were assessed using in situ hyperspectral  $R_{rs}$  representative of diverse water types. Excluding waters dominated by a high concentration of colored dissolved organic matter, results indicate the capability of determining hyperspectral  $R_{rs}$ from AERONET-OC multispectral data with mean relative and absolute uncertainties generally lower than 2% and  $5 \times 10^{-5}$  sr<sup>-1</sup>, respectively, at a number of the key center-wavelengths of the Ocean Color Instrument (OCI) onboard the Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) spacecraft.

Index Terms-Ocean color, remote sensing, validation.

#### I. INTRODUCTION

ATELLITE-DERIVED remote sensing reflectance R<sub>rs</sub> of natural waters has shown fundamental relevance to investigate marine ecosystems through retrieved information on optically significant water constituents such as phytoplankton concentration. This was achieved through multispectral data across a number of satellite sensor including the Sea-viewing Wide Field-of-view Sensor (SeaWiFS [1]) up to the recent Ocean and Land Color Instrument (OLCI [2]).

Further advances in satellite ocean color applications, likely benefitting of a robust determination and quantification of phytoplankton species, are expected by the exploitation of data from hyperspectral sensors like those operated by the Italian Space Agency on the PRecursore IperSpettrale della Missione Applicativa (PRISMA) [3] or by the National Aeronautics and

Manuscript received 20 October 2023; accepted 3 January 2024. Date of publication 8 January 2024; date of current version 22 January 2024. This work was supported in part by the "Severo Ochoa Center of Excellence" Accreditation under Grant CEX2019-000928-S and in part by the National Aeronautics and Space Administration (NASA) through the Goddard Earth Sciences Technology and Research (GESTAR) II Award under Grant 80NSSC22M0001. The work of Jaime Pitarch was supported by the European Union through the NextGenerationEU Program, Italian Integrated Environmental Research Infrastructures System (ITINERIS) Project. (Corresponding author: Marco Tallone.)

Marco Talone is with the Departament de Oceanografía Física i Tecnològica and the Barcelona Expert Center (BEC), Institut de Ciències del Mar Space Administration on the forthcoming Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) [4].

The increased spectral resolution and number of satellite sensors bands, however, require adequate in situ reference measurements for a comprehensive validation of derived radiometric data products. This implies access not only to in situ measurements exhibiting suitable spatio-temporal coverage, but also satisfying the uncertainty requirements allowing to verify the fitness-for-purpose of satellite-derived radiometric products at the relevant center-wavelengths. This need urges advancements on those satellite validation methods still relying on multispectral data such as those from the Ocean Color component of the Aerosol Robotic Network (AERONET-OC) [5]. As an alternative to the exclusive use of hyperspectral sensor data (e.g., those from WATER-HYPERNET [6]) to support the validation of satellite hyperspectral radiometric products, this work addresses the potential for applying multispectral data without restricting the process to the sole matching spectral bands. This effort is justified by: 1). the evidence that a finite number of spectral  $R_{rs}$  values allows for reconstructing the full  $R_{rs}$  spectrum, still at the expense of a decreased accuracy (e.g., [7], [8]); 2) the assumption that a relatively small increase in the uncertainty of reconstructed  $R_{rs}$  values away from the actual in situ center-wavelengths might still ensure basis for a satisfactory exploitation of these data in the validation of satellite ocean color radiometric products; and 3) the outstanding maturity of the AERONET-OC network that, established in 2002, benefits of high standardization of instruments and measurement methods [5], unique investigations on instruments performance [9] and measurement uncertainties [10], extensive efforts to verify the accuracy of radiometric products [11], and consolidated data reduction and quality control schemes [12].

The main objective of the study is the quantification of the uncertainties characterizing reconstructed  $R_{\rm rs}$  at PACE ocean color center-wavelengths solely relying on AERONET-OC multispectral data from diverse water types.

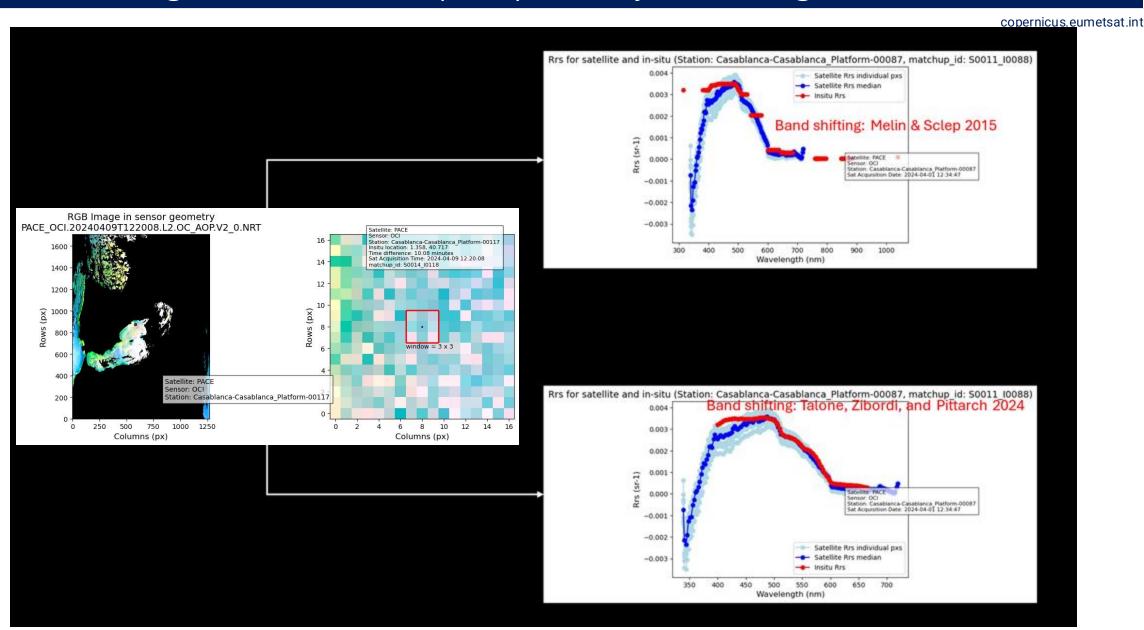
II. DATA AND METHODS

A. R<sub>rs</sub> Center-Wavelengths

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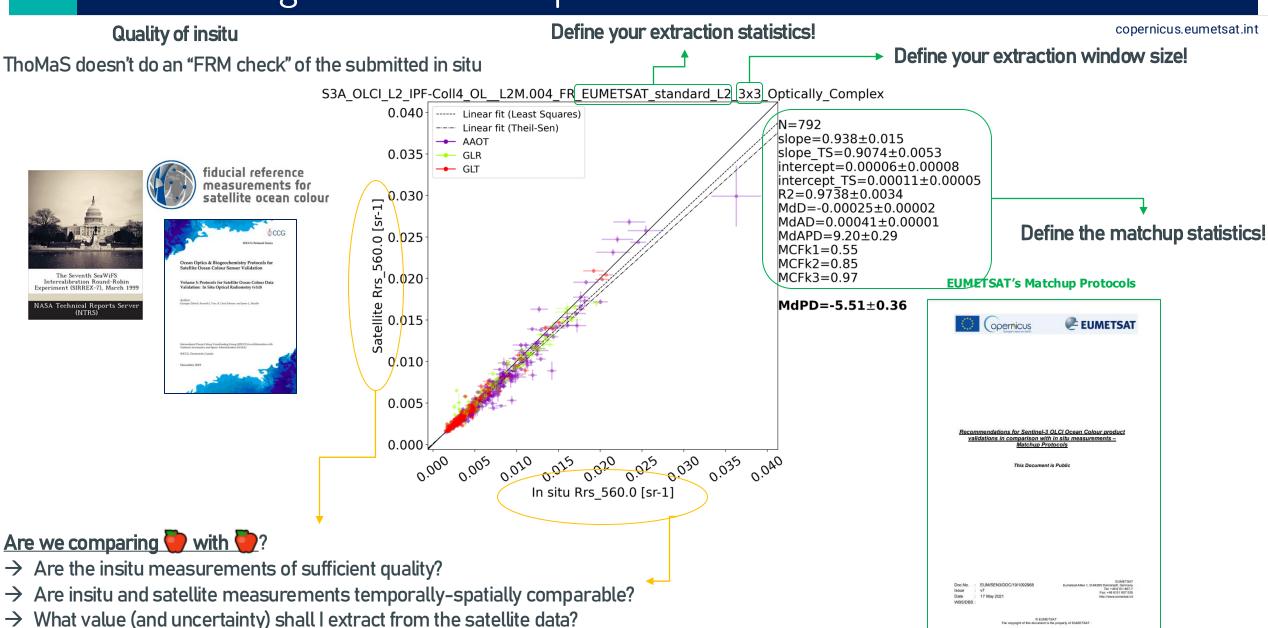


## Some background: match-ups (spectrally matching insitu to satellite)



#### 2

#### Some background: match-ups

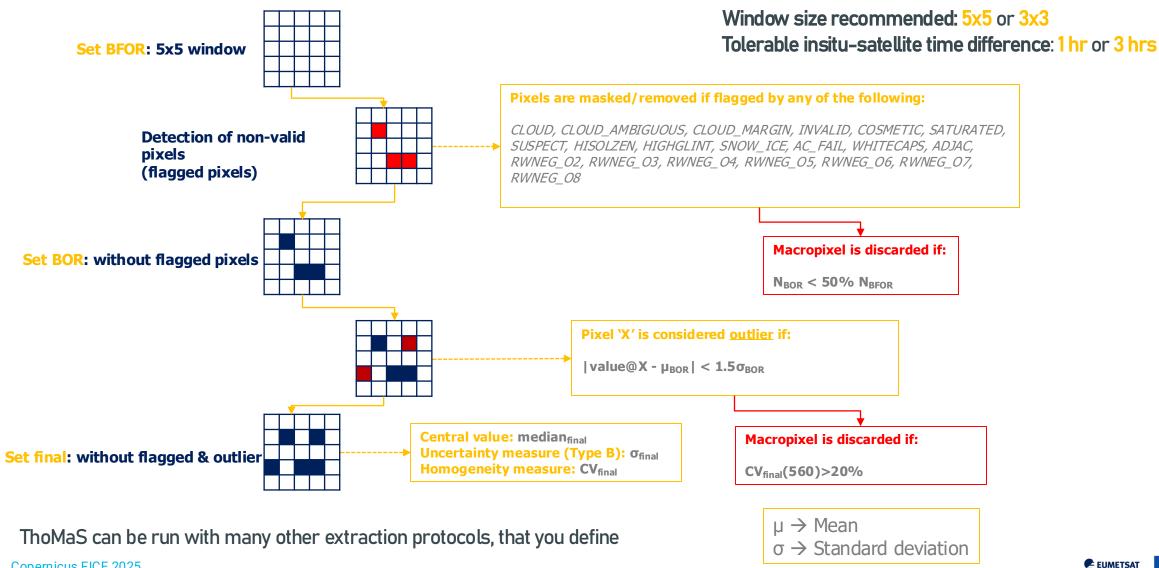




### Some background: match-ups: EUMETSAT extraction protocol

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#### **EUMETSAT's Matchup Protocols:** extraction of statistics at macropixel level



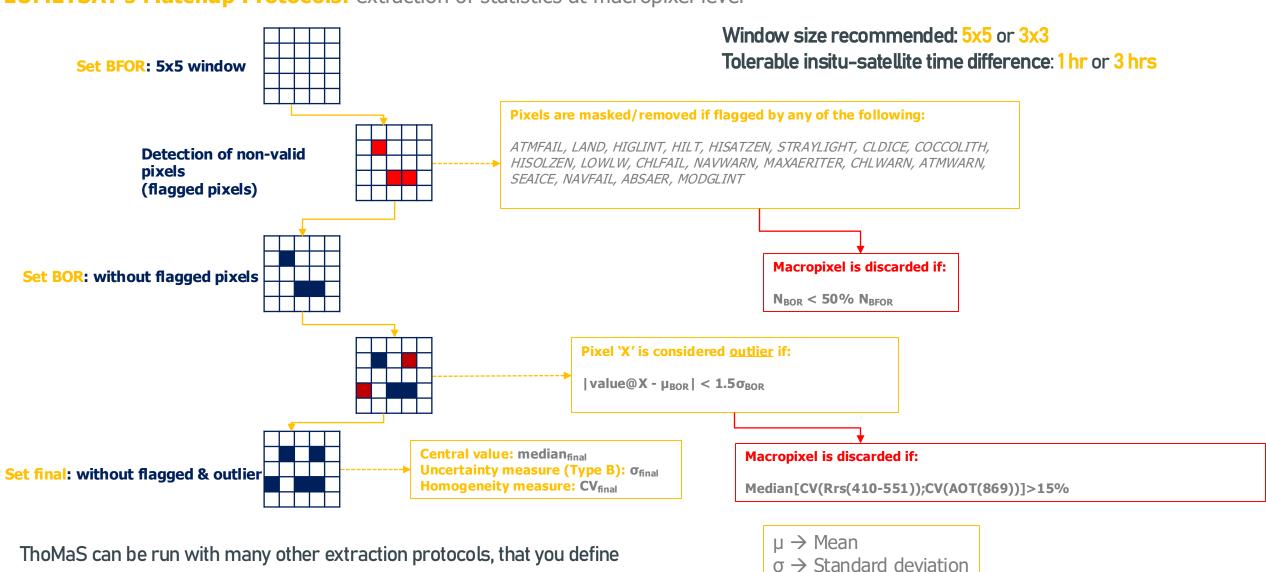
**EUMETSAT** 



## Some background: match-ups: Bailey & Werdell protocol

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**EUMETSAT's Matchup Protocols:** extraction of statistics at macropixel level



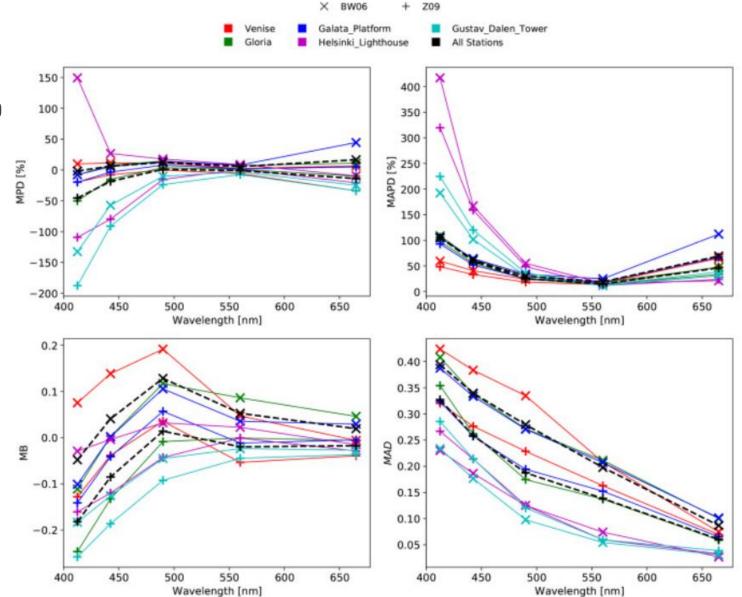
**EUMETSAT** 

# Some background: match-ups: what protocol to use?

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Should we care ab

YES

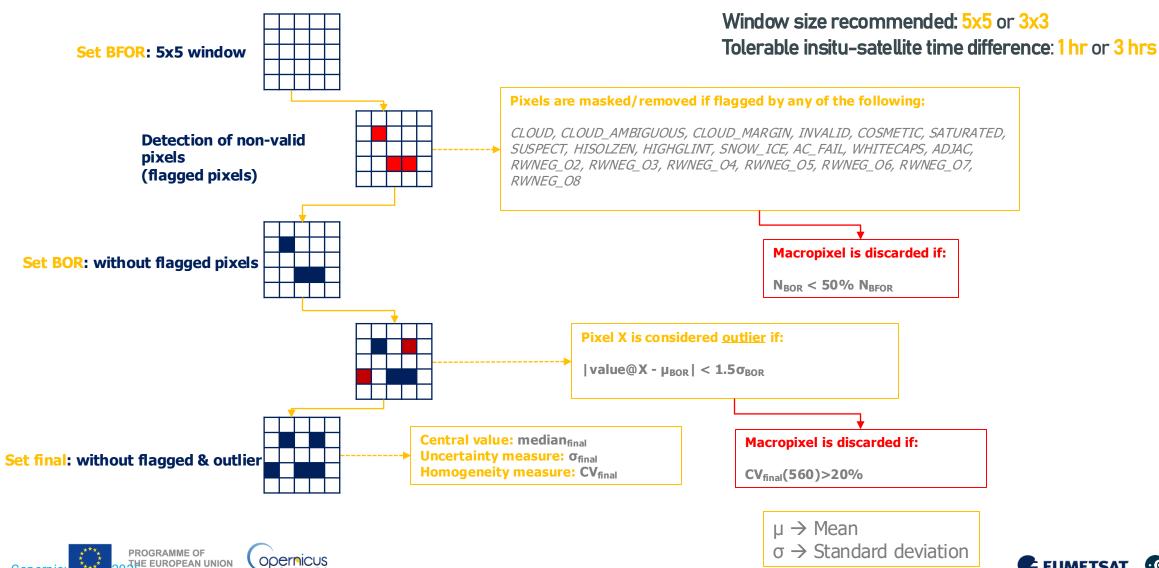


[Concha et al. 2021]

#### Current EUMETSATs matchup protocol

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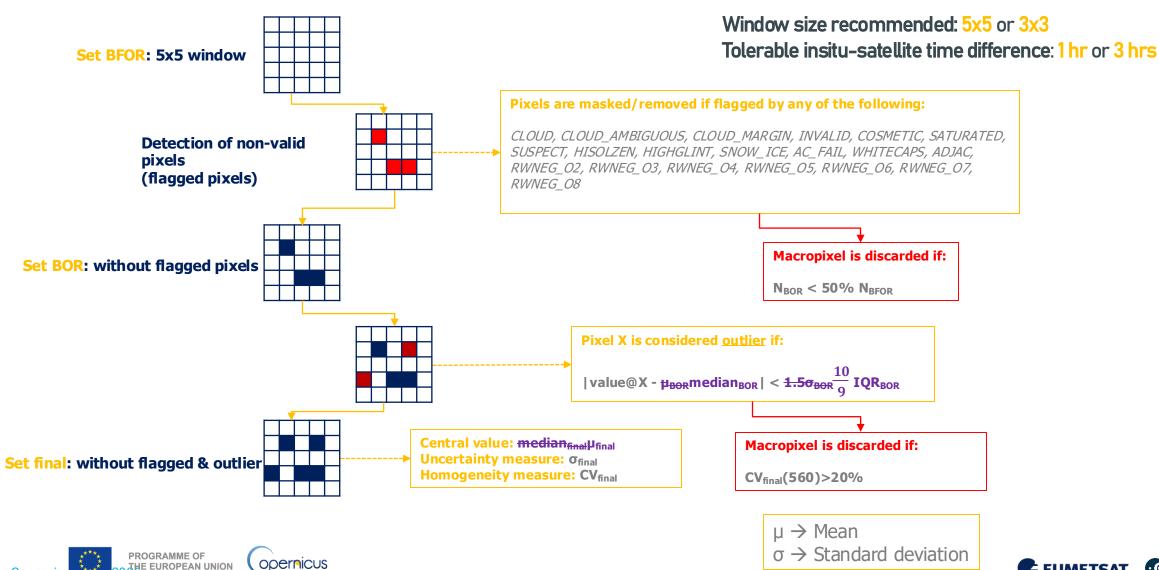
**EUMETSATs Matchup Protocols:** extraction of statistics at macropixel level



## Current EUMETSATs matchup protocol: proposed changes (1)

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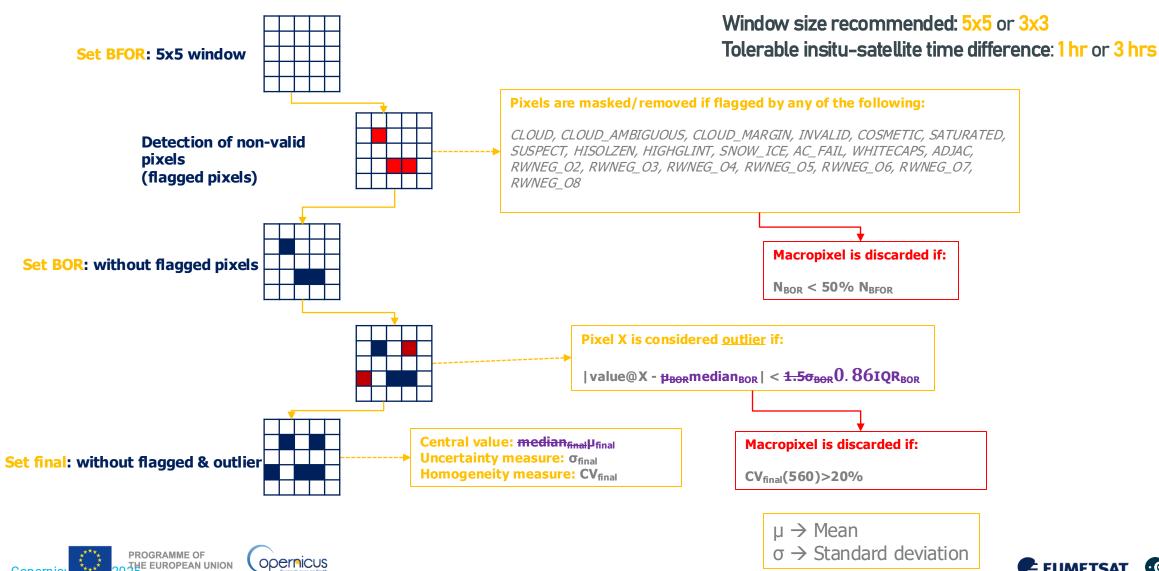
**EUMETSATs Matchup Protocols:** extraction of statistics at macropixel level



## Current EUMETSATs matchup protocol: proposed changes (2)

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**EUMETSATs Matchup Protocols:** extraction of statistics at macropixel level



- In situ data used: AERONET-OC, Level 2.0
- Stations: Casablanca\_Platform, Gloria, Helsinki\_Lighthouse, LISCO, Section-7\_Platform, USC\_SEAPRISM, Galata\_Platform, Gustav\_Dalen\_Tower, Lake\_Erie, Palgrunden, Socheongcho, Venise
- A total of 2139 matchups



## Comparing outlier detection, pixel by pixel

copernicus.eumetsat.int

#### Proposed "1"

Pixel X is considered outlier if:

 $|value@X - median| < \frac{10}{9} \times IQR$ 

Central value = mean

NOT OUTLIEFE

#### Current protocol

Pixel X is considered <u>outlier</u> if:  $|value@X - mean| < 1.5 \times \sigma$  Central value = median

OTHER

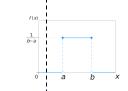
88.4% 3.27% 1.35% 7.02%

#### Proposed "2"

Pixel X is considered <u>outlier</u> if:

 $|value@X - median| < \frac{\sqrt{3}}{2} \times IQR$ 

Central value = mean



#### Current protocol

Pixel X is considered <u>outlier</u> if:  $|value@X - mean| < 1.5 \times \sigma$  Central value = median

83.5% 8.06% 2.32% 8.14%







## Comparing screened macropixels

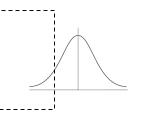
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#### Proposed "1"

Pixel X is considered outlier if:

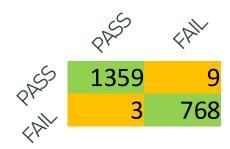
$$|value@X - median| < \frac{10}{9} \times IQR$$

Central value = mean



#### Current protocol

Pixel X is considered <u>outlier</u> if: |value@X - mean|  $< 1.5 \times \sigma$ Central value = median

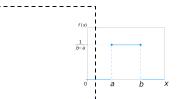


#### Proposed "2"

Pixel X is considered outlier if:

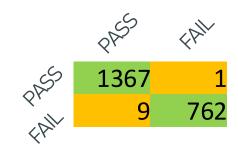
$$|value@X - median| < \frac{\sqrt{3}}{2} \times IQR$$

Central value = mean

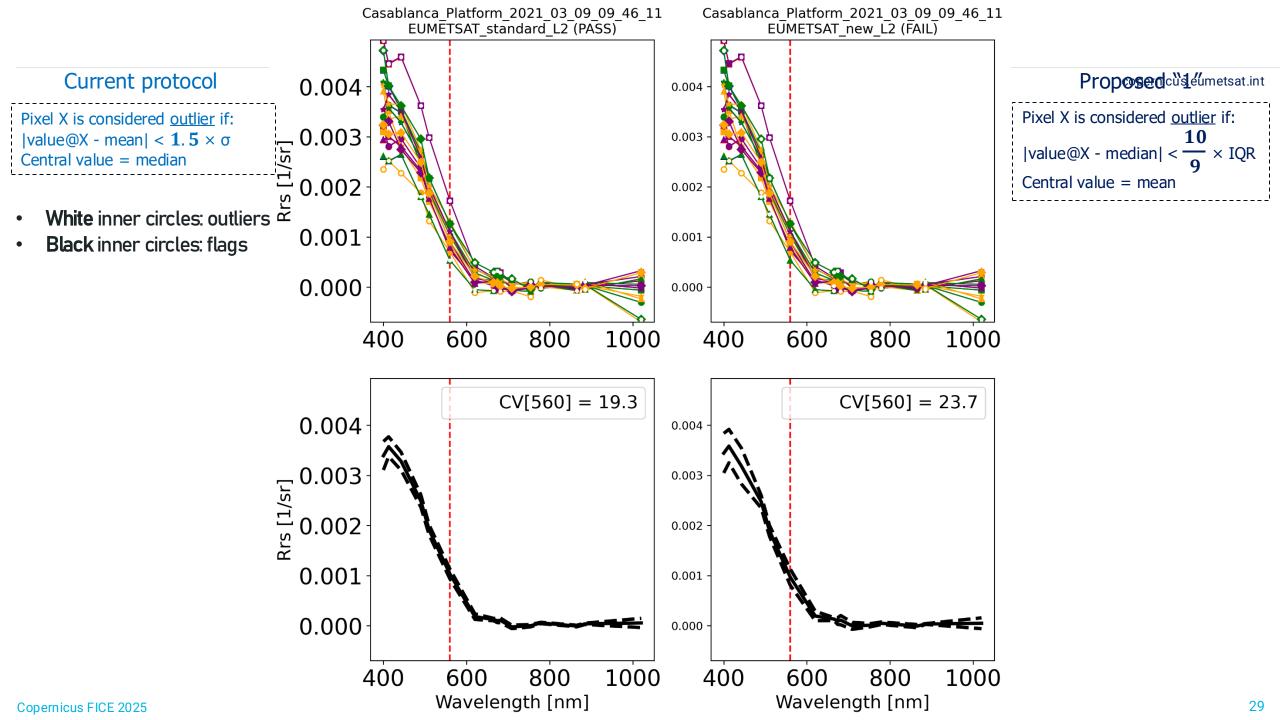


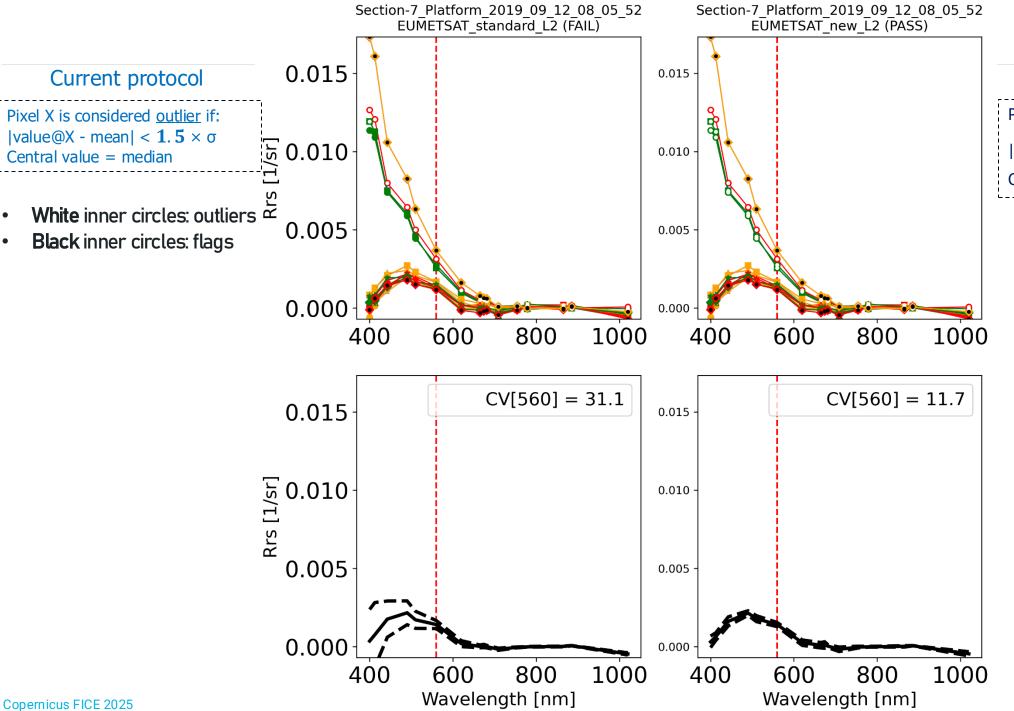
#### Current protocol

Pixel X is considered <u>outlier</u> if: |value@X - mean|  $< 1.5 \times \sigma$ Central value = median







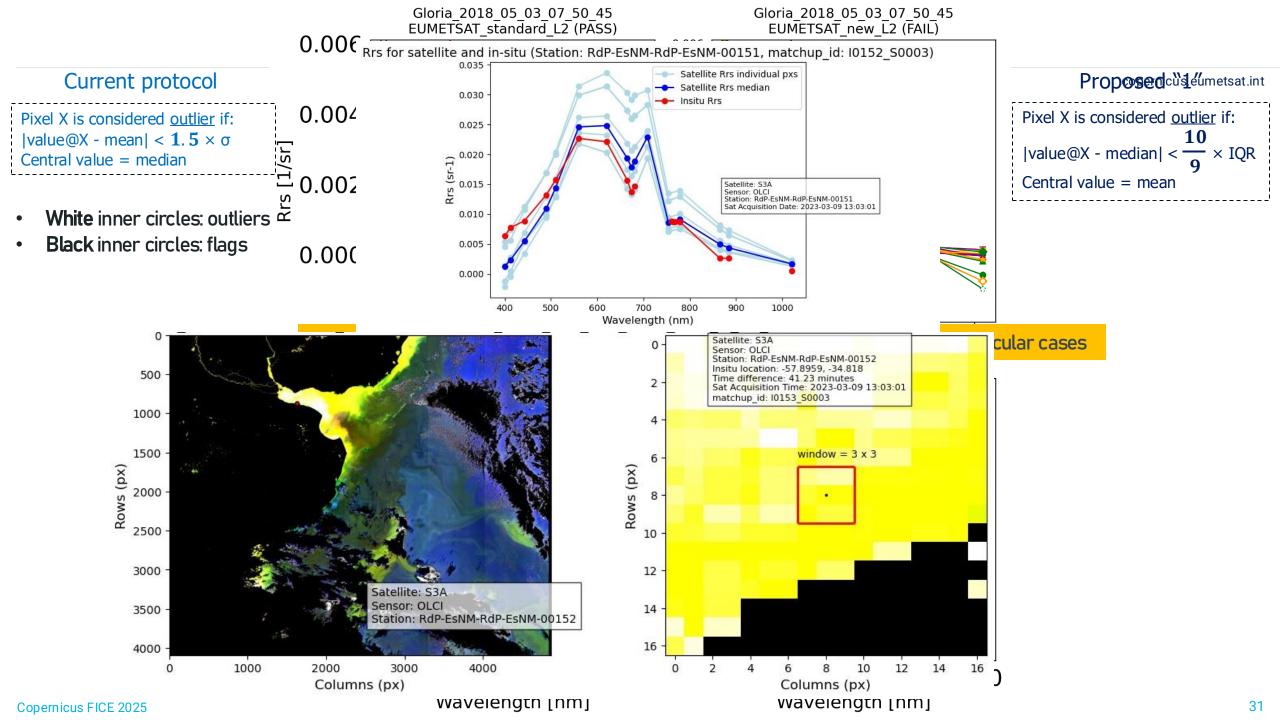


Proposedcust eumetsat.int

Pixel X is considered <u>outlier</u> if:

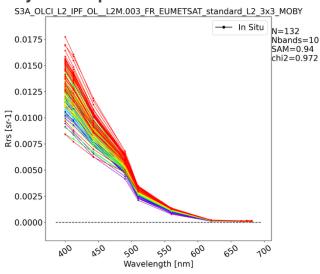
**10**  $|value@X - median| < \frac{1}{9} \times IQR$ 

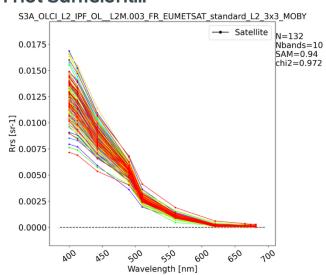
Central value = mean

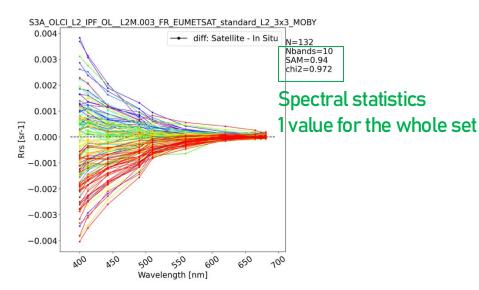


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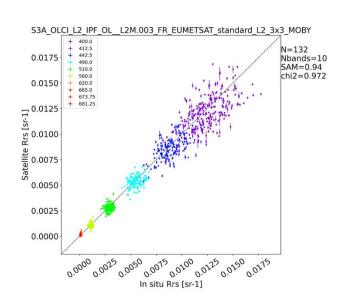
#### Band-by-band plots and statistics are often not sufficient...

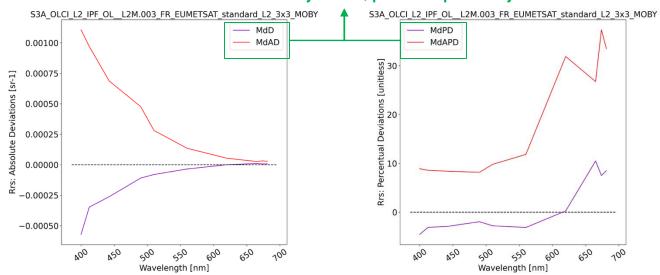






#### statistics band-by-band, plotted spectrally

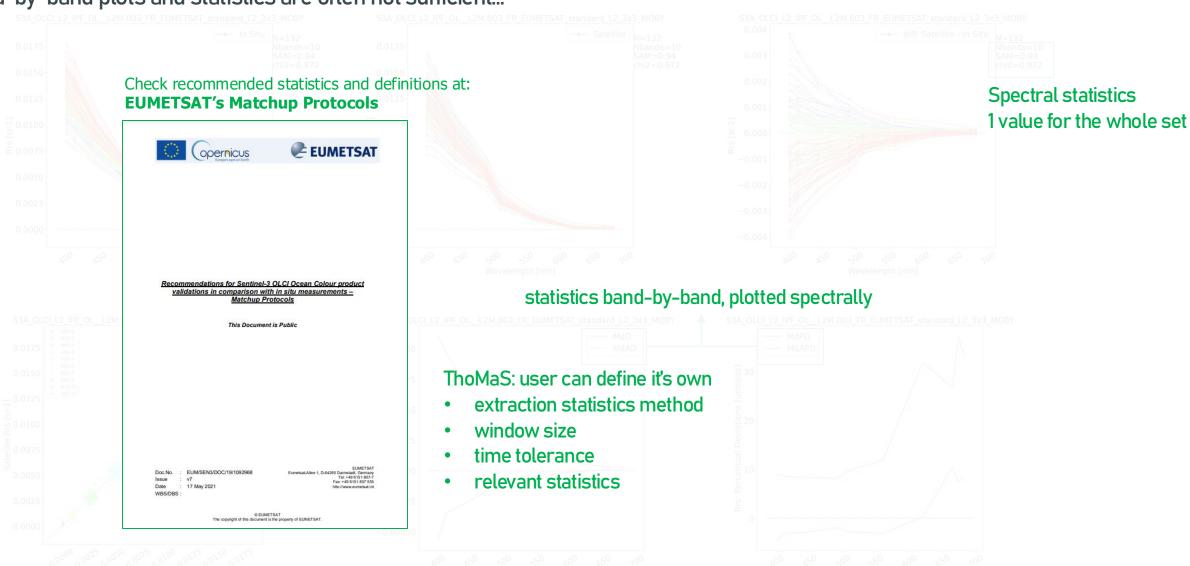






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Band-by-band plots and statistics are often not sufficient...



#### Some background: match-ups, performance metrics used

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Mean Difference →

$$\frac{1}{n}\sum_{i=1}^{n} \left\{ Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i} \right\}$$

Mean Percent Difference →

$$\frac{1}{n}\sum_{i=1}^{n} \left\{ \frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i}}{Rrs(\lambda)_{in \, situ,i}} \right\}$$

Mean Absolute Difference →

$$\frac{1}{n} \sum_{i=1}^{n} \{ |Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i} | \}$$

Mean Absolute Percent Difference →

$$\frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{|Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i}|}{Rrs(\lambda)_{in \, situ,i}} \right\}$$

Log-based Mean Absolute Difference  $\rightarrow LogMAD_{\lambda} = 10^{\sum_{i=1}^{N} |log_{10}(Rrs(\lambda)o_{LCI,i}) - log_{10}(Rrs(\lambda)in situ,i)|}$ 

### Some background: match-ups, performance metrics used

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Median Difference →

$$\operatorname{median}_{1 \le i \le N} \left\{ Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i} \right\}$$

Median Percent Difference →

$$\operatorname{median}_{1 \le i \le N} \left\{ \frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i}}{Rrs(\lambda)_{in \, situ,i}} \right\}$$

Median Absolute Difference →

$$\underset{1 \le i \le N}{\operatorname{median}} \{ |Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \ situ,i} | \}$$

Median Absolute Percent Difference →

$$\operatorname{median}_{1 \le i \le N} \left\{ \left| \frac{Rrs(\lambda)_{OLCI,i} - Rrs(\lambda)_{in \, situ,i}}{Rrs(\lambda)_{in \, situ,i}} \right| \right\}$$

## Some background: match-ups, performance metrics used

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Spectral Angle Mapper →

$$SAM = \frac{1}{N} \sum_{i=1}^{N} \left( acos \left( \frac{\langle Rrs_{in \, situ,i}, Rrs_{OLCI,i} \rangle}{\left\| Rrs_{in \, situ,i} \right\| \left\| Rrs_{OLCI,i} \right\|} \right) \right)$$

Chi-squared →

$$\chi^{2} = \frac{1}{N} \sum_{i=1}^{N} \left( \sum_{\lambda} \frac{\left( Y(\lambda)_{in \, situ,i} - Y(\lambda)_{OLCI,i} \right)^{2}}{Y(\lambda)_{in \, situ,i}} \right)$$

$$Y(\lambda)_i = \frac{Rrs(\lambda)_i}{Rrs(560)_i}$$

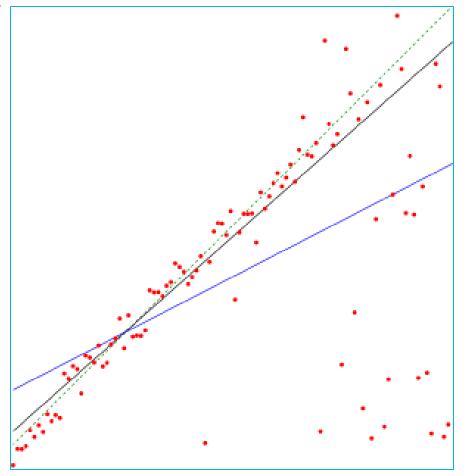
+ linear regression of two types...



## Some background: match-ups, performance metrics used

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+ linear regression of two types...



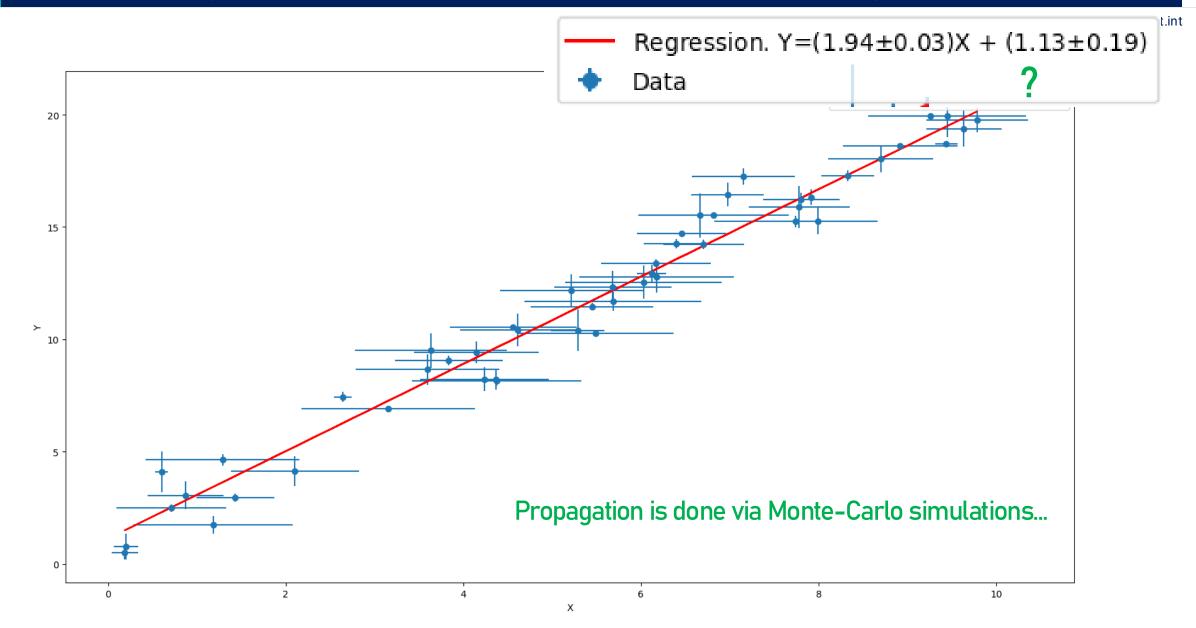
--- Standard Least-Squares

---Theil-Sen regressor

- 1:1 line

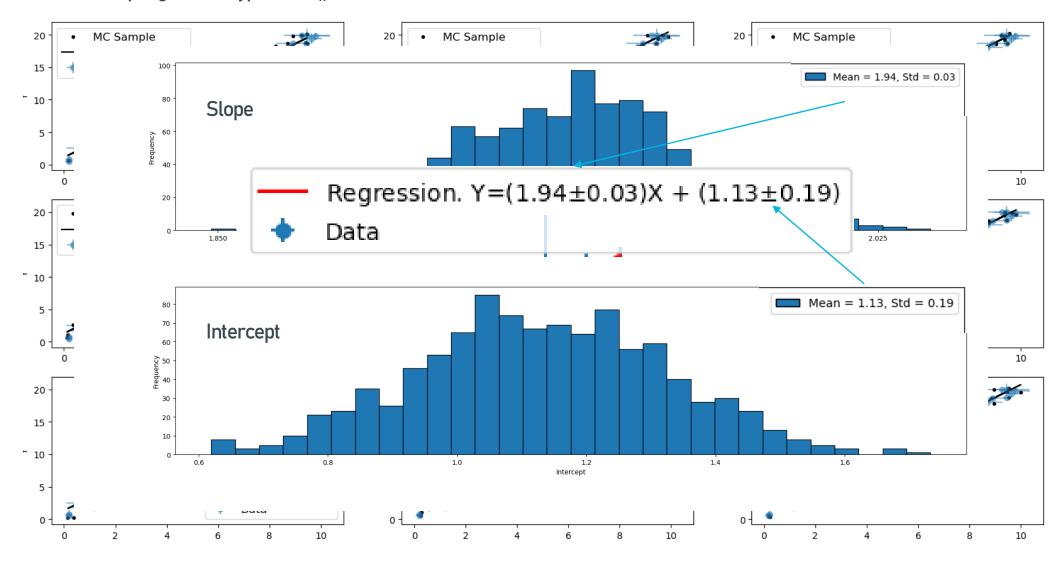
There is no one better than the other. Having both to compare can give a first assessment of the effect of the outliers in your matchup performanaces





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1000 random re-samplings of the type  $N(x,u_x)$ 

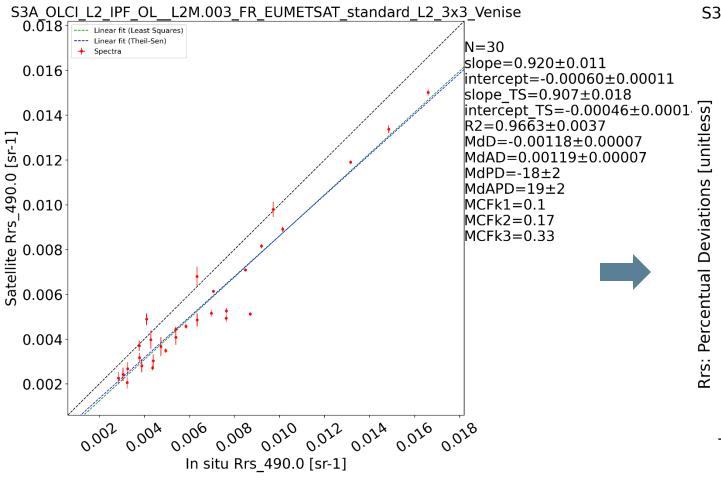


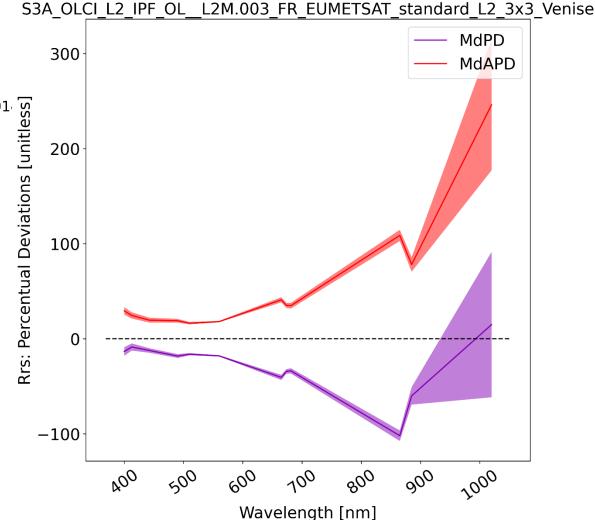
copernicus.eumetsat.int

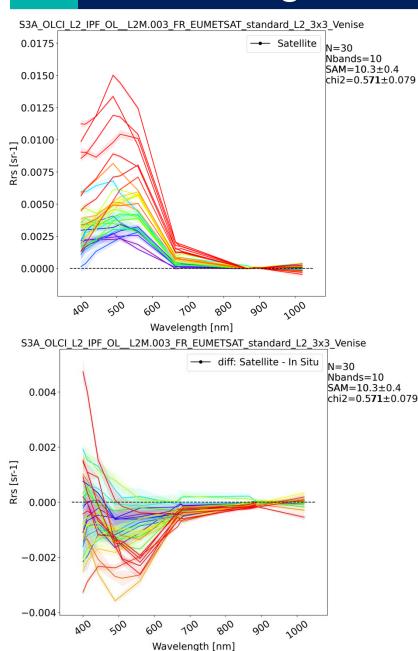
#### Uncertainties in satellite/insitu component ...

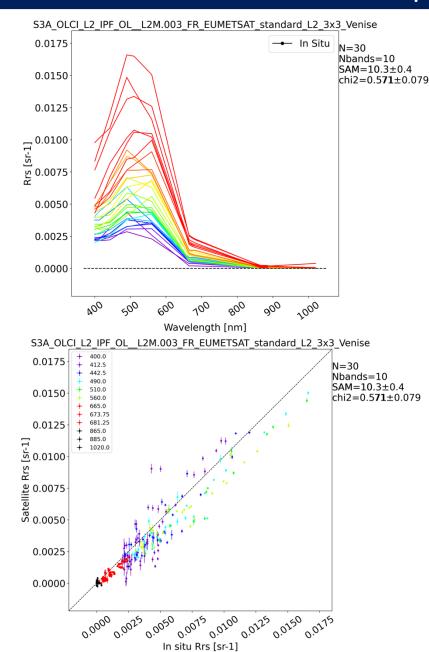


#### ... propagated to performance metrics





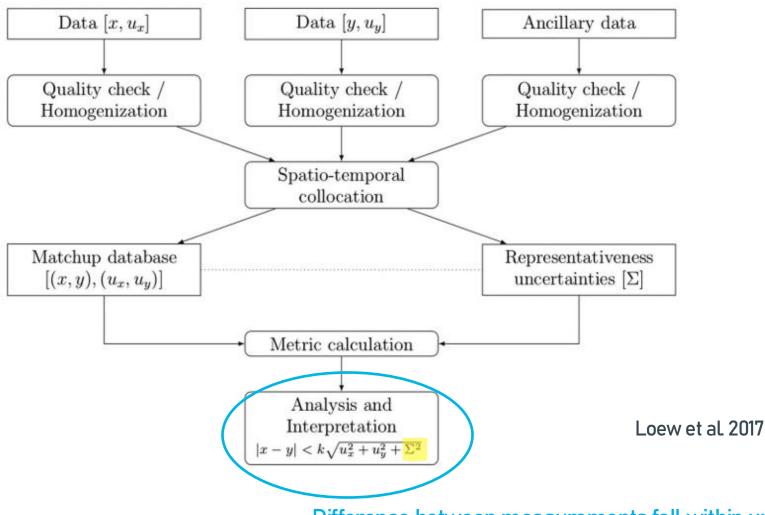






# Some background: Metrologically-Compatible Fraction

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Difference between measurements fall within uncertainties?

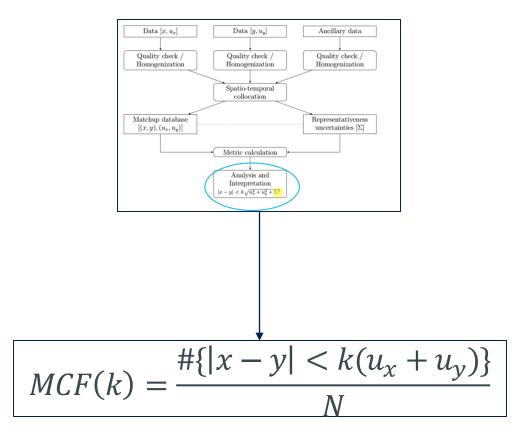
k = coverage factor

**E** EUMETSAT

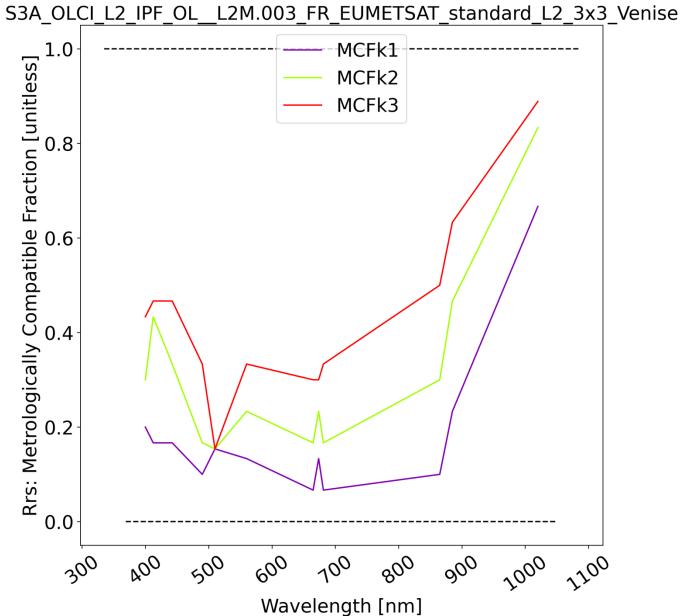


## Some background: Metrologically-Compatible Fraction

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Metrologically-Compatible Fraction
→ Recommended by Kevin Ruddick



Copernicus FICE 2025



#### A discussion slide: are radar plots providing a "master performance metric"?

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#### Area of a radar plot, the definite statistics?

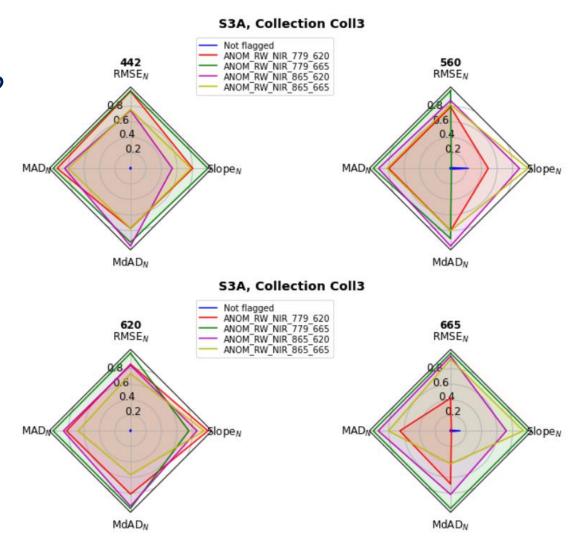
All performance metrics are mathematical calculations entirely based on your data.

But they have a concrete meaning.

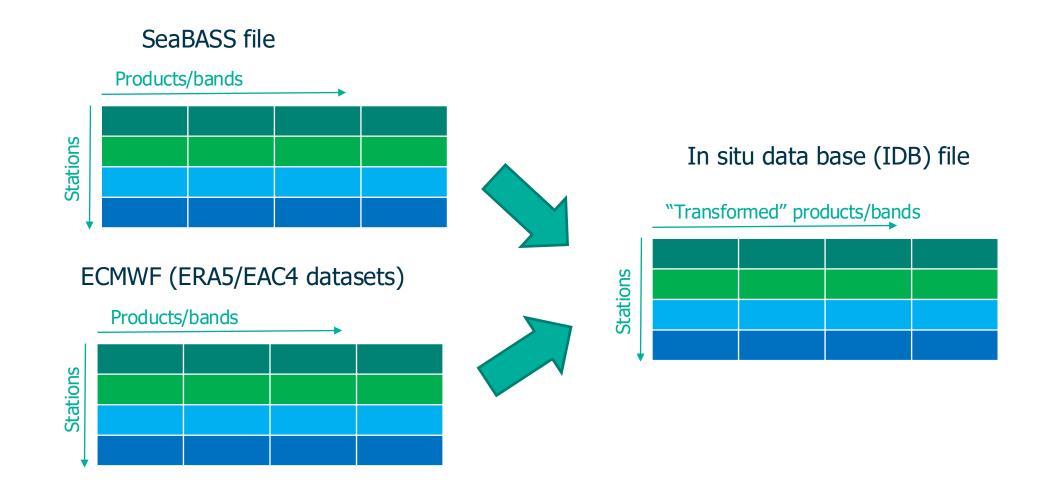
The area inside the radar plot is ambiguous in two senses:

- It depends on the (typically random) way in which you normalize the axes.
- It depends on the \*typically random) choice of statistics that represent each vertex

In the end, it's just a soup of sums and subtractions of other performance metrics that have a specific justification for being defined as they are..





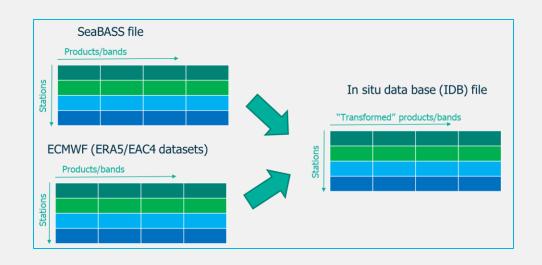




### Usage. Step insitu: SeaBASS/OCDB file

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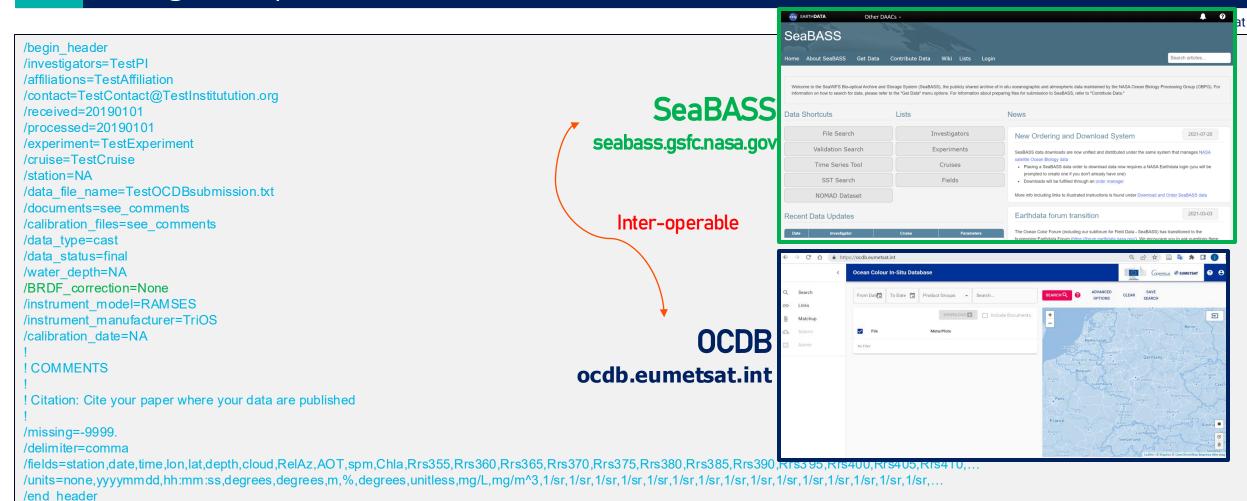


#### /end header

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#### Usage. Step insitu: SeaBASS/OCDB file



 $Test Station 001, 20210815, 11:30:00, 0, 0, 0.01, 0, 134.7, 0.2444, 0.1, 0.1, 0.001886946, 0.002068008, 0.002167035, 0.002305759, 0.002504616, 0.002699149, 0.002943716, 0.003166, \dots \\ Test Station 001, 20210815, 11:30:00, 0, 0, 0.01, 0, 134.7, 0.2444, 0.1, 0.1, 0.001886946, 0.002068008, 0.002167035, 0.002305759, 0.002504616, 0.002699149, 0.002943716, 0.003166, \dots \\ Test Station 001, 20210815, 11:30:00, 0, 0, 0.01, 0, 134.7, 0.2444, 0.1, 0.1, 0.001886946, 0.002068008, 0.002167035, 0.002305759, 0.002504616, 0.002699149, 0.002943716, 0.003166, \dots \\ Test Station 001, 20210815, 11:30:00, 0, 0, 0.01, 0, 134.7, 0.2444, 0.1, 0.1, 0.001886946, 0.002068008, 0.002167035, 0.002305759, 0.002504616, 0.002699149, 0.002943716, 0.003166, \dots \\ Test Station 001, 20210815, 2021$ TestStation002,20201014,11:55:00,-32.6232,32.0859,0.01,0.134.8,0.2388,0.1,0.1,0.002158972,0.002363762,0.00247761,0.00264967,0.002880799,0.003116844,0.0034196,...  $Test Station 003, 2020 1014, 12:16:00, -32.0209, 26.9584, 0.01, 0, 134.7, 0.2388, 0.1, 0.1, 0.001918189, 0.002097384, 0.002191946, 0.002353893, 0.002567901, 0.002792078, 0.00307, \dots$ TestStation004,20210910,09:40:00,3,-3,0.01,0,134.9,0.2388,0.1,0.1,0.001271305,0.001359205,0.00139314,0.001432681,0.001487187,0.00153414,0.00160502,0.00165816,...

 $Test Station 005, 20210910, 09:54:00, -4,4,0.01,0,134.8,0.277,0.1,0.1,0.00123858, 0.001313013, 0.001336158, 0.00136599, 0.001412448, 0.001450581, 0.001508596, 0.00155277, \dots$  $Test Station 006, 20210910, 10:07:00, 5, -5, 0.01, 0, 134.8, 0.277, 0.1, 0.1, 0.001126482, 0.001192422, 0.001211226, 0.001237373, 0.001276362, 0.001307301, 0.00135953, 0.0013975, \dots$ 

**EUMETSAT** 



#### Usage. Step insitu: SeaBASS/OCDB file

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/affiliations=TestAffiliation
/contact=TestContact@TestInstitutution.org
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/processed=20190101
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/cruise=TestCruise
/station=NA
/data file name=TestOCDBsubmission.txt
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/calibration files=see comments
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/BRDF correction=M02
/instrument model=RAMSES
/instrument manufacturer=TriOS
/calibration date=NA
! COMMENTS
! Citation: Cite your paper where your data are published
/missing=-9999.
/delimiter=comma
```

You can use Excel to bring your data to this format...
However...

 $TestStation 001, 20210815, 11:30:00, 0, 0, 0.01, 0, 134.7, 0.2444, 0.1, 0.1, 0.001886946, 0.002068008, 0.002167035, 0.002305759, 0.002504616, 0.002699149, 0.002943716, 0.003166, \dots \\ TestStation 002, 20201014, 11:55:00, -32.6232, 32.0859, 0.01, 0, 134.8, 0.2388, 0.1, 0.1, 0.002158972, 0.002363762, 0.00247761, 0.00264967, 0.002880799, 0.003116844, 0.0034196, \dots \\ TestStation 003, 20201014, 12:16:00, -32.0209, 26.9584, 0.01, 0, 134.7, 0.2388, 0.1, 0.1, 0.001918189, 0.002097384, 0.002191946, 0.002353893, 0.002567901, 0.002792078, 0.00307, \dots \\ TestStation 004, 20210910, 09:40:00, 3, -3, 0.01, 0, 134.8, 0.277, 0.1, 0.001271305, 0.001359205, 0.00139314, 0.001432681, 0.001487187, 0.00153414, 0.00160502, 0.00165816, \dots \\ TestStation 005, 20210910, 09:54:00, -4, 4, 0.01, 0, 134.8, 0.277, 0.1, 0.1, 0.00123858, 0.001313013, 0.001336158, 0.00136599, 0.001412448, 0.001450581, 0.001369953, 0.0013975, \dots \\ TestStation 006, 20210910, 10:07:00, 5, -5, 0.01, 0, 134.8, 0.277, 0.1, 0.1, 0.001126482, 0.001192422, 0.001211226, 0.001237373, 0.001276362, 0.001307301, 0.00135953, 0.0013975, \dots \\ TestStation 006, 20210910, 10:07:00, 5, -5, 0.01, 0, 134.8, 0.277, 0.1, 0.1, 0.001126482, 0.001192422, 0.001211226, 0.001237373, 0.001276362, 0.001307301, 0.00135953, 0.0013975, \dots \\ TestStation 006, 20210910, 10:07:00, 5, -5, 0.01, 0, 134.8, 0.277, 0.1, 0.001126482, 0.001192422, 0.001211226, 0.001237373, 0.001276362, 0.001307301, 0.00135953, 0.0013975, \dots \\ TestStation 006, 20210910, 10:07:00, 5, -5, 0.01, 0, 134.8, 0.277, 0.1, 0.1, 0.001126482, 0.001192422, 0.001211226, 0.001237373, 0.001276362, 0.001307301, 0.00135953, 0.0013975, \dots \\ TestStation 006, 20210910, 10:07:00, 5, -5, 0.01, 0, 134.8, 0.277, 0.1, 0.001126482, 0.001192422, 0.001211226, 0.001237373, 0.001276362, 0.001307301, 0.00135953, 0.0013975, \dots \\ TestStation 006, 20210910, 10:07:00, 5, -5, 0.01, 0.0145074, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474, 0.001237474,$ 

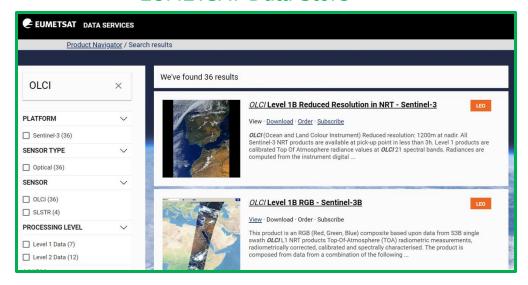
AutoSave ( 20210916\_Ana[ Usage. Step ins ile – editing with Excel... Page Lavout Formulas  $\equiv$ Calibri copernicus.eumetsat.int 20210916 AnaDelgado.sb - Notepad Paste ≣ File Edit Format View Help 20210916\_AnaD-ThoMaS deals with these ... /begin header /investigators=Ana Lau Clipboard File Edit Format View Help  $\overline{}$ Font /affiliations=Institut/ /begin\_header,,,,, Text Import Wizard - Step 1 of 3 /contact=aldelgado@iad /investigators=Ana Laura Delgado,,,,, /begin\_header The Text Wizard has determined that your data is Fixed Wid /experiment=Monte Herm /affiliations=Instituto Argentino de Oceanografia..... /cruise=Pescadores /contact=aldelgado@iado-conicet.gob.ar,,,,, If this is correct, choose Next or choose the data type that b E F G H I /documents=lom.2012.10n /begin\_header /experiment=Monte\_Hermoso,,,,, Text Import Wizard - Step 1 Original data type linvestigators=Ana Laura Delgado /calibration files=NA /cruise=Pescadores,,,,, l'affiliations=Instituto Argentino de Oceanografia Choose the file type that bes This screen lets you set the de 3 /data\_type= bottle /documents=lom.2012.10.1011,,,, /contact=aldelgado@iado-conicet.gob.ar Delimited - Char /data\_status=final /calibration\_files=NA,,,,, lexperiment=Monte Hermoso Delimiters /water depth= 0 Fixed width - Field /data\_type= bottle,,,,, /cruise=Pescadores Tab /wavelength option=NA /documents=lom.2012.10.1011 /data\_status=final,,,,, Semicolon - 8 Icalibration files=NA /instrument\_model=NA /water depth= 0,,,, /data\_type= bottle Start import at row: 1 Comma /instrument manufactur5 /wavelength\_option=NA,,,,, Te:10 /data\_status=final Space /instrument\_model=NA,,,, /calibration date=NA 11 /water depth= 0 /cloud percent=NA Other: 12 /wavelength\_option=NA /instrument manufacturer=NA,,,,, My data has headers. 13 /instrument model=NA /secchi depth=NA /calibration\_date=NA,,,,, 14 /instrument manufacturer=NA /wave\_height=NA /cloud percent=NA,,,, 15 /calibration date=NA /wind speed=NA /secchi\_depth=NA,,,,, Preview of file C:\Users\Gos: 16 /cloud percent=NA /wave height=NA,,,, 17 /secchi depth=NA 1/begin\_header 2/investigators=Ana 3/affiliations=Inst-COMMENTS Data preview 18 /wave height=NA /wind\_speed=NA,,,, 19 /wind\_speed=NA ! For this cruise, Tot<sup>5</sup> !,,,,, 4/contact=aldelgadc 5/experiment=Monte 6/cruise=Pescadorec 7/documents=lom.201 20 ! Water samples were f ! COMMENTS,,,,, /begin\_header COMMENTS For this Total Suspended Matter was sourced from surface water samples taken wCDB > 20210916\_Ana\_De! For this cruise, Total Suspended Matter was sourced from surface water samples taken wCDB > 20210916\_Ana\_De! ! The optimal filtered affiliations=Insti ! The Whatman GF/F fil -! Water samples were filtered immediately after the extraction following  $^{\circ}$ Water samples were filtered immediately after the extraction following the protocol of ! pre-weighed and rins /experiment=Monte\_F24 ! The op ranging from 0.51 to 21 ! The optimal filtered volume was determined according to the obtained tur /cruise=Pescadores /documents=1om.201,25 ! The Whatman GF/F filters used were pre-combusted at 500 ŰC for 4 hours ! The filters were ond ! The Whatman GF/F filters used were pre-combusted at 500 °C for 4 hours pre-weil and dried at 65 ŰC until a constant weight was observed. pre-weighed and rinsed with at least 250 ml milli-Q water to eliminate : The filters were once more weighed before the filtrations occurred. ! The filters were once more weighed before the filtrations occurred.,,,, 28 Add a Place /missing=-999. !,,,,, 29 /delimiter=comma .30 /missing=-999. !,,,,, ne current file type. 31 Idelimiter=comma /fields=time,lat,lon,station,spm,date /missing=-999.,,,, 32 /fields=tillat station /units=hh:mm:ss,degrees,degrees,none,mg/L,yyyymmdd /delimiter=comma,,,,, 33 /units=hi dearees dearees none ma/L yyyymmdd /fields=time,lat,lon,station,spm,date /end header 34 lend header 14:30:00, -38.790, -62.280, 1, 156, 20170901 156 2E+07 /units=hh:mm:ss,degrees,degrees,none,mg/L,yyyymmdd 14:30:00 -38.79 -62.28 12:20:00 -62.22 32 2E+07 /end\_header,,,,, -38.799 -62.264 49 2E+07 12:55:00 14:30:00,-38.79,-62.28,1,156,20170901 -62.331 47 2E+07 14:30:00 -38,775 -62,331 75 2E+07 14:15:00 -38.742 42 2E+07 -38,751 -62.383 -38.864 28 2E+07 15:00:00 16:00:00 -38.888 -62.19 36 2E+07 34 2E+07 17:00:00 -38.89 -62,191 44 18:00:00 -38.882 -62,201 31 2E+07 19:00:00 -38.864 -62.216 37 2E+07 -38.79 84.1 2E+07 -62.28 13:00:00 51.5 2E+07 13:30:00 -38.79 -62.28 58.4 14:00:00 -38.79 -62.28 2E+07 15:00:00 -38.79 -62.28 135.4 2E+07 -38.79 -62.28 412.3 2E+07 50 16:00:00

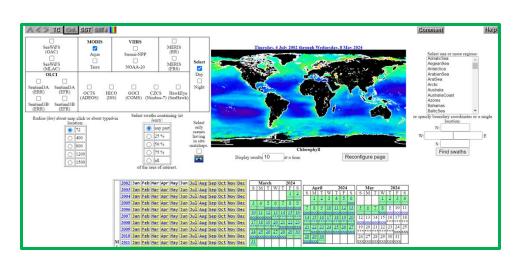


### Usage. Step SatData

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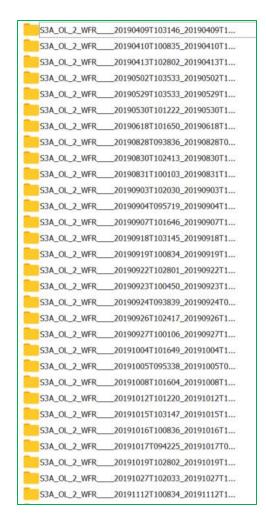
#### **EUMETSAT Data Store**







#### Your local system

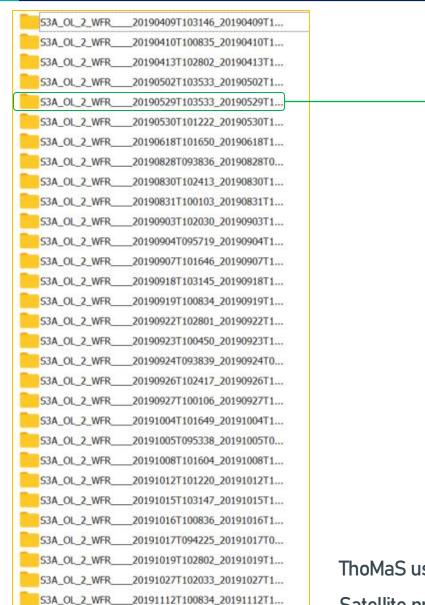


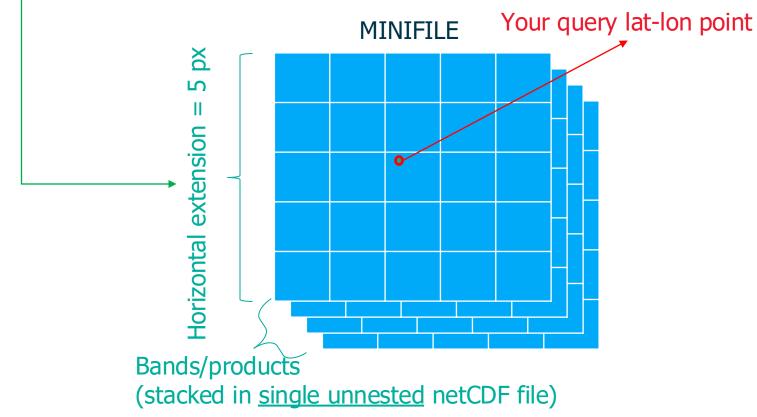
#### + SatData Lists matching in situ



#### Usage. Step minifiles

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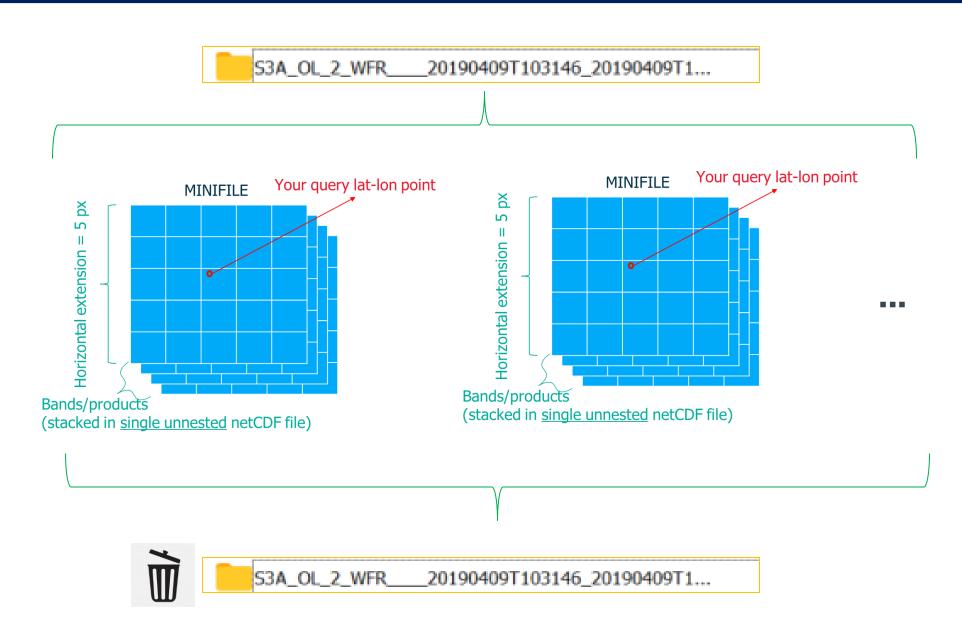




ThoMaS uses the minimisation of the orthodromic distance approach to find the centroid of the window Satellite products are not altered at all at this step, with the exception of some OLCI geometries...



# Usage. Option download\_extract\_delete



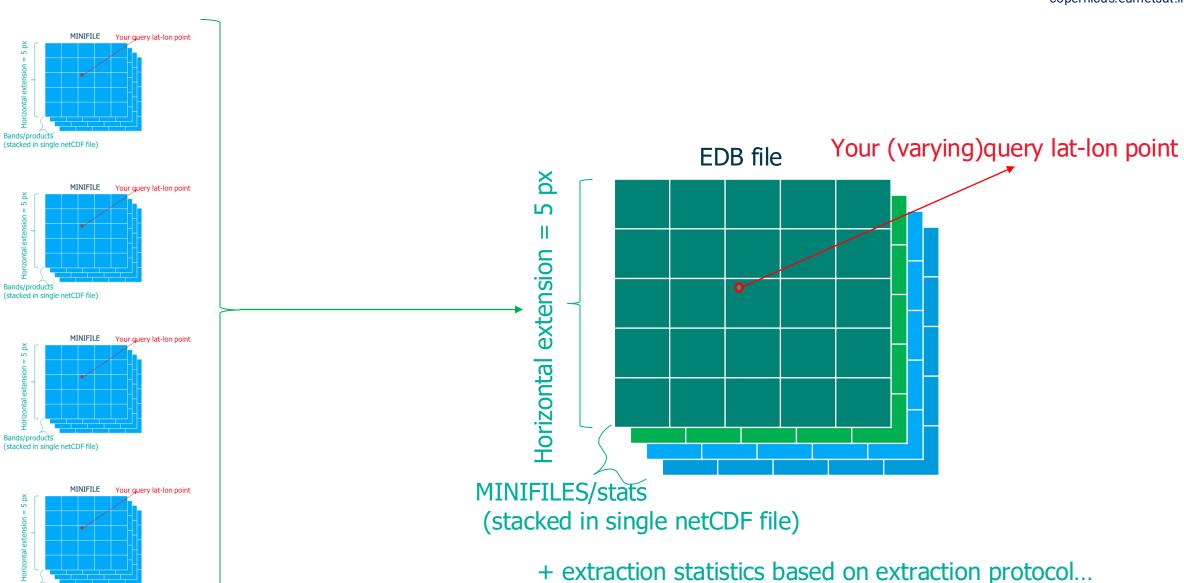


### EOCanvas Cloud Based Processing of EO data: ThoMaS and S3/OLCI



### Usage. Step EDB

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Operaicus

Bands/products (stacked in single netCDF file)

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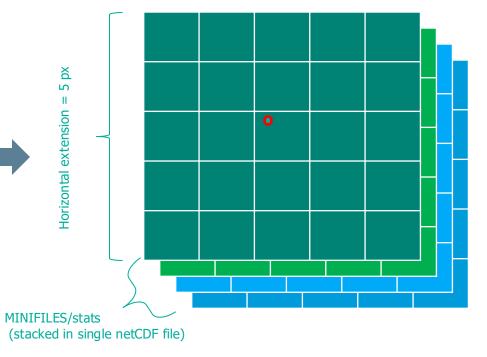
#### **MDB** file

- 1. Merging insitu and extractions according to matchup pairs
- 2. Statistical metrics calculated + scatter/spectral plots

In situ data base (IDB) file

Products/bands

MDB: indexed by matchup pair ID Time interpolation (nearest in time) applicable Extraction data base (EDB) file



### Pre-requisites

- Apart from that background knowledge...
- 2. Install the latest Anaconda Python distribution.
- 3. Install git





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#### Git way:

cd ~ mkdir ThoMaS cd ThoMaS git clone --depth 1 https://gitlab.eumetsat.int/eumetlab/oceans/ocean-science-studies/ThoMaS.

#### Direct download:

https://gitlab.eumetsat.int/eumetlab/oceans/ocean-science-studies/ThoMaS

Recent updates were done on the code

git pull



#### Setting the environment

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 Once conda and ThoMaS are installed, create the thomas env:



libmamba is the best choice for those of you who are stuck in the "Solving environment step"



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- 1. EUMETSAT Data Store/OBPG credentials obtained and stored?
- 2. (optional) ECMWF ADS/CDS credentials obtained and stored?
- 3. ThoMaS code cloned?
- 4. thomas conda environment set up and activated?
- 5. Required inputs in place? (config\_file.ini, insitu input file?)

If **YES**.. run by executing this command: python /path/to/ThoMaS/main.py -cf /path/to/config\_file.ini

Or to run in GUI mode: python /path/to/ThoMaS/main.py

